Supplementary Material

Table S1. Experimental Inhibitory concentration 50% (IC_{50}) of TAN against MBLs from bibliography.

MBL	IC_{50} (µM)	Ref.
NDM-1	0.1	1
NDM-9	53	1
NDM-30	17	2
VIM-2	0.04	1
VIM-2 Glu149Lys	46	1
VIM-83	80	2
IMP-1	>100	1
SIM-1	>100	2

1. Le Terrier C, Gruenig V, Fournier C, Nordmann P, Poirel L. 2023. NDM-9 resistance to taniborbactam. Lancet Infect Dis 23:401–402.

2. Le Terrier C, Viguier C, Nordmann P, Vila AJ, Poirel L, submitted for publication.

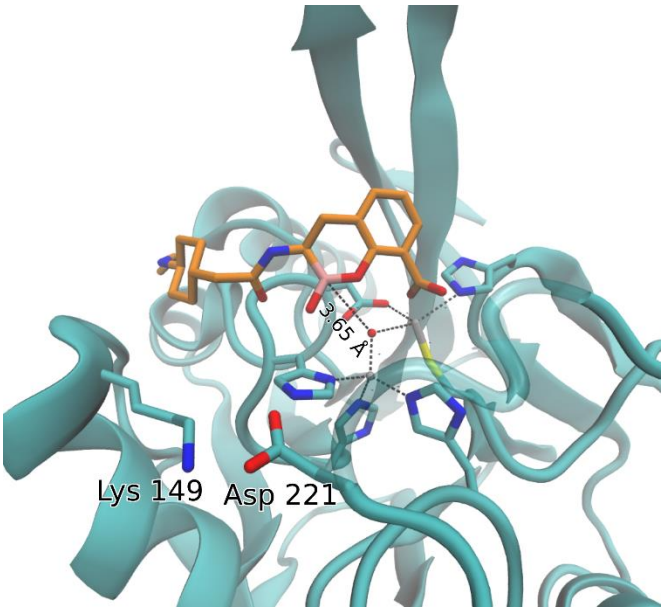

Figure S1. Second most populated pose found in the docking simulation results for TAN with NDM-9. For visual clarity, hydrogen atoms are omitted.

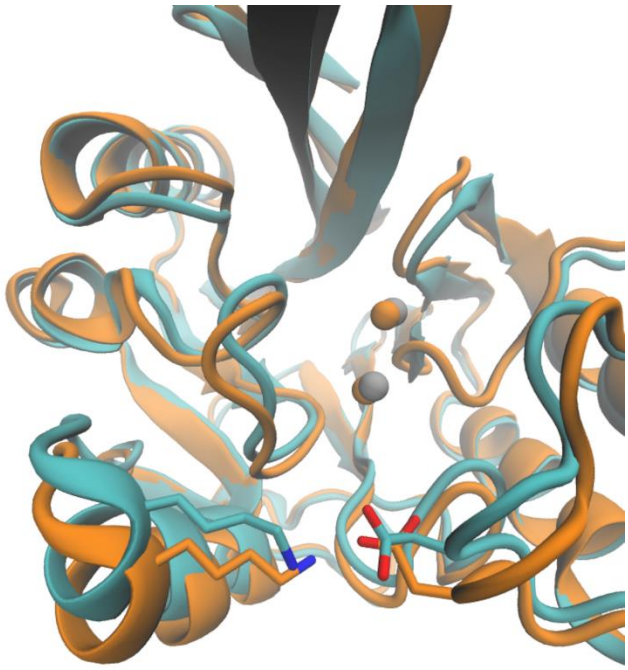

Figure S2. Superposition of the NDM-9 crystallographic structure (C atoms in cyan, Zn atoms in gray) and the most representative conformation (C and Zn atoms in orange) of the cluster of conformations explored during the molecular dynamics simulation.

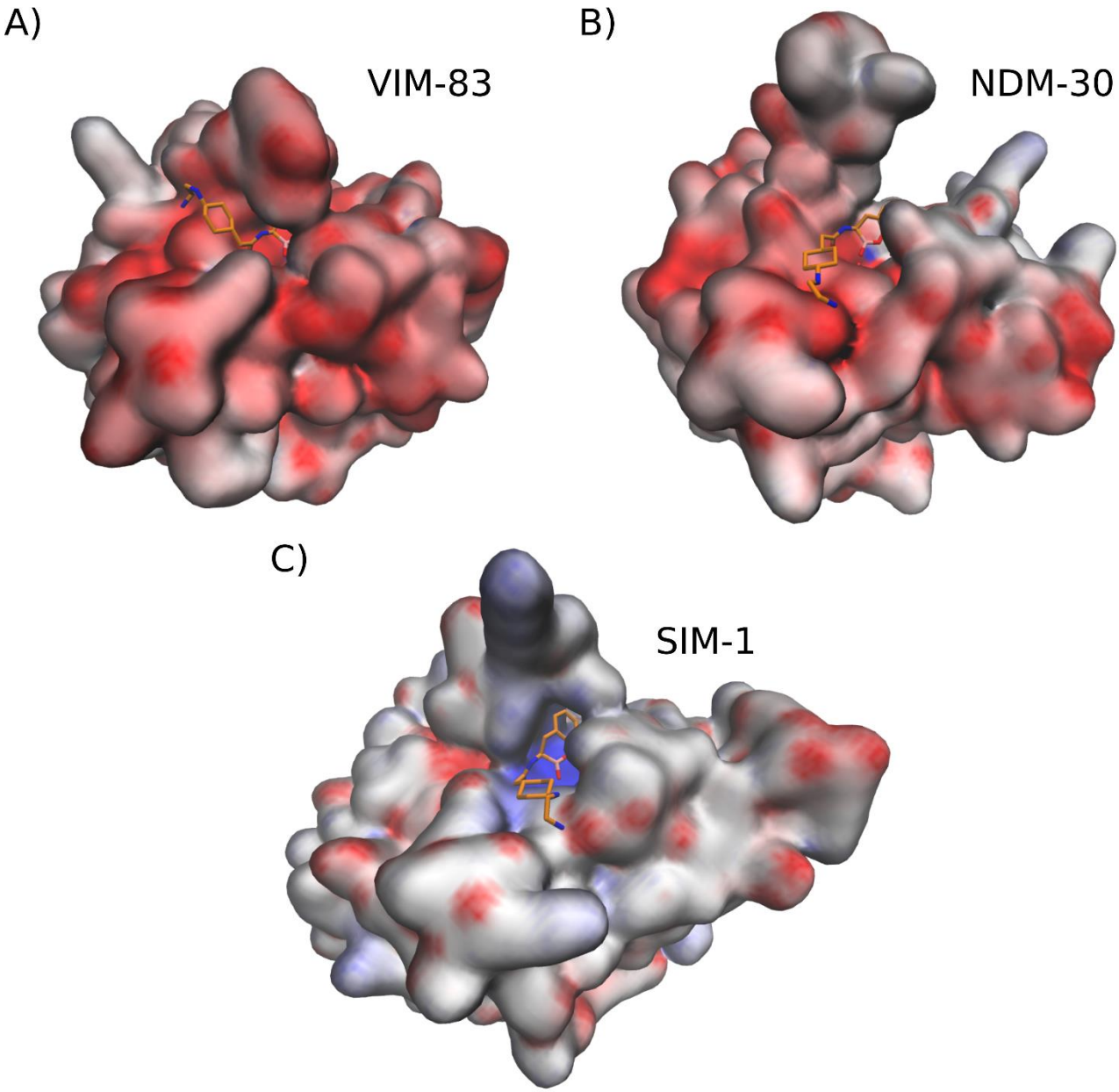

Figure S3. Electrostatic potential surfaces of proteins of A) VIM-83, B) NDM-30 and C) SIM-1. The productive pose of the docking experiments of TAN to each protein are also shown (C atoms of TAN are depicted in orange). Negative, neutral and positive potentials are colored as red, white and blue respectively, in a scale from -10 to 10 k_BT/e_c.